A BIOENGINEERED MEMORY STORAGE DEVICE USING BACTERIORHODOPSIN AND GRAPHENE

Romaben Patel[1], Amanda Petrus[2] and Isaac Macwan[1]
[1]Department of Biomedical Engineering, University of Bridgeport
[2]Department of Chemistry, University of Bridgeport

ABSTRACT

Bacteriorhodopsin (BR) is a photoactive protein, which has been studied as a memory storage device owing to its photochemical and thermal stability[1]. BR photocycle comprises of two distinct stable binary states, bR (0) and Q (1) based on the wavelength of the applied radiation[2]. However, such devices have a limited success due to low quantum yield of the Q state[1]. Many studies have used genetic and chemical modification as optimization strategies to increase the yield of the Q state compromising the overall photochemical stability of the BR[1]. Here we come up with a unique way of stabilizing the conformations of BR and thereby the BR and Q states of the protein through its adsorption onto graphene. We have used all-atom molecular dynamics (MD) simulations utilizing NAMD (Nanoscale Molecular Dynamics) and the CHARMM (Chemistry at HARvard Macromolecular Mechanics) force field to understand the interactive events at the interface of BR and a single layer graphene sheet. Based on the stable RMSD (Root Mean Square Deviation) and interactive energies such as Van-der-Waals and electrostatics, we propose that the adsorption of BR onto graphene can stabilize the photochemical behavior of BR. Furthermore, the switching between Cis and Trans conformations of the retinal based on the angular change of the dihedral demonstrates that such an adsorption is beneficial to preserve the binary states.

METHOD

Molecular Dynamics

- PDB file of native bacteriorhodopsin (BR) protein (1AT9) was used to create its .psf file using VMD[3].
- An inbuilt graphene builder was used to create a graphene sheet of 100Å × 100Å.
- A TCL script is used to adjust a distance of 7Å between graphene and protein.
- TIP3P[4] water model and neutralizing salt concentration were setup using VMD and simulations were carried out using NAMD[5] for 75ns.
- All-atom simulations used CHARMM[6] force field and the boundary conditions were assumed, using a constant temperature of 300K and a pressure of 1 atm.
- 1500 steps of energy minimization were performed first to stabilize the system followed by 1ns of equilibration.
- Interaction energies (Van-der-Waals and electrostatics), RMSD and salt bridges were analyzed using VMD.

RESULTS

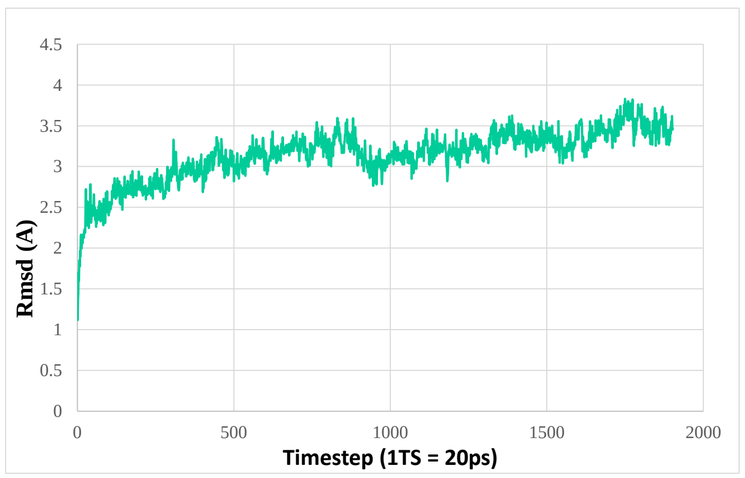

Figure 1: RMSD plot

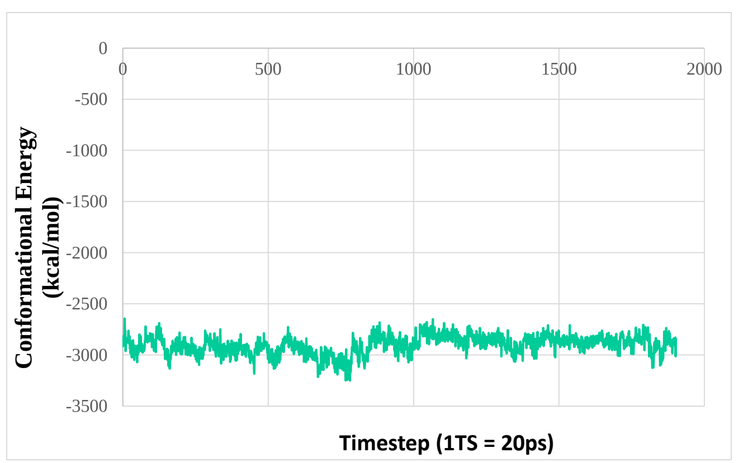

Figure 2: Total Conformational energy

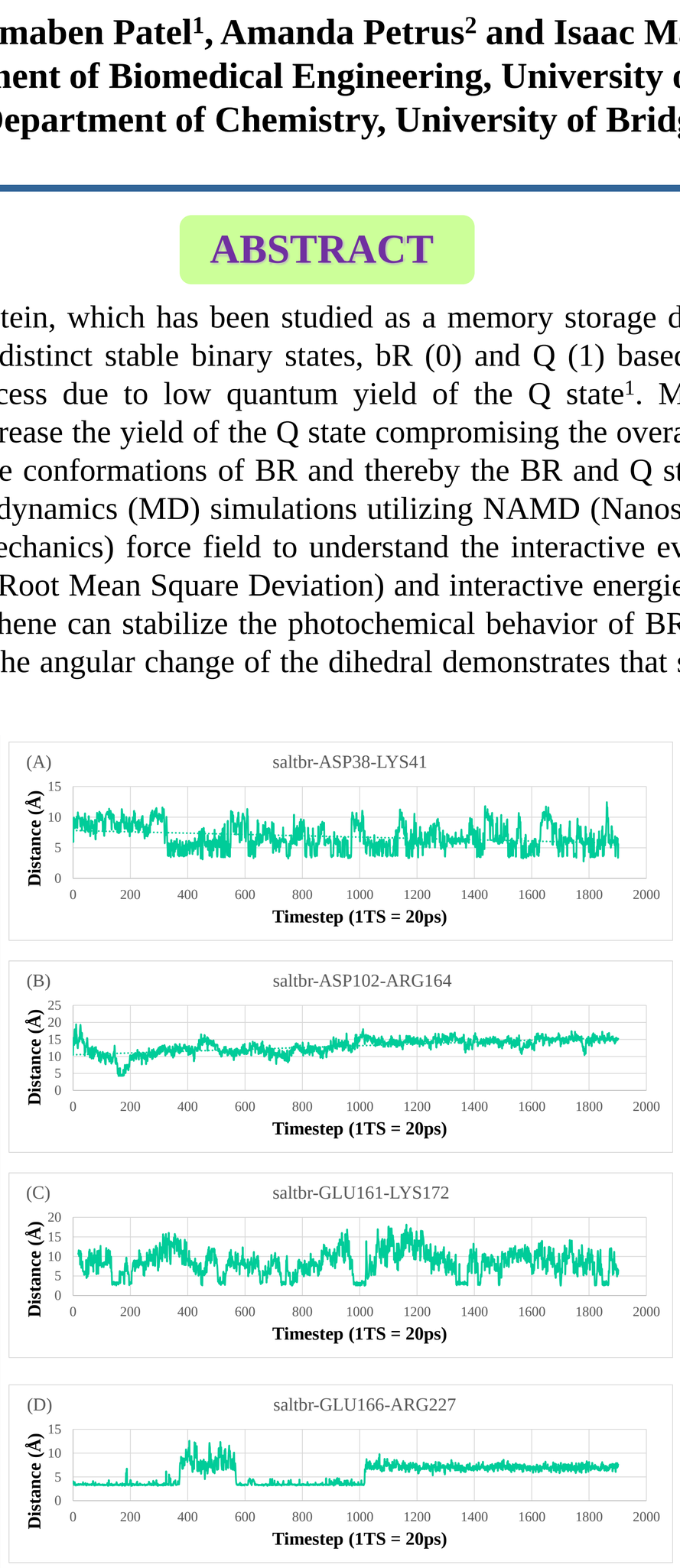

Figure 3 (A), (B), (C), and (D): Protein Salt Bridges at BR protein – Graphene interaction site.

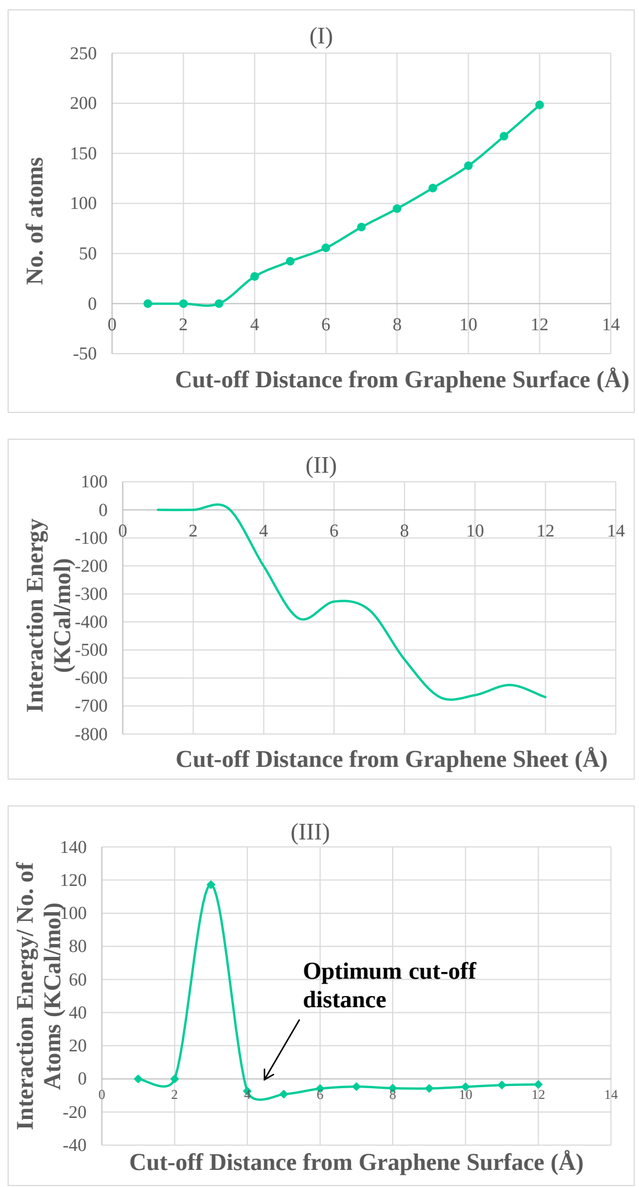

Figure 4 (I), (II), (III): Analysis of interaction between BR protein and Graphene

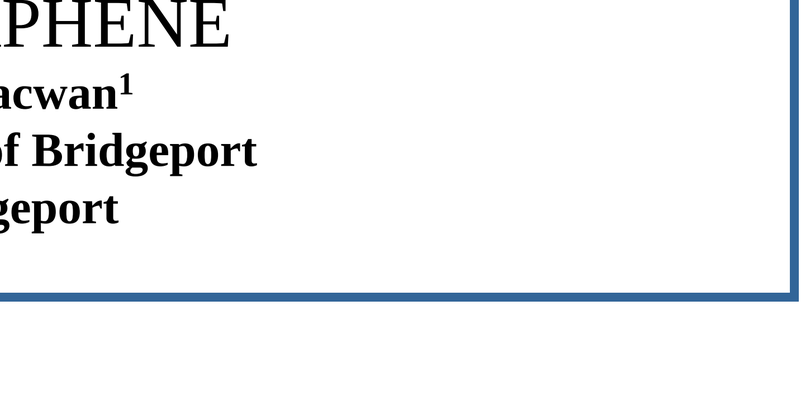

Figure 5: Number of H bonds within 5 Å of retinal active site

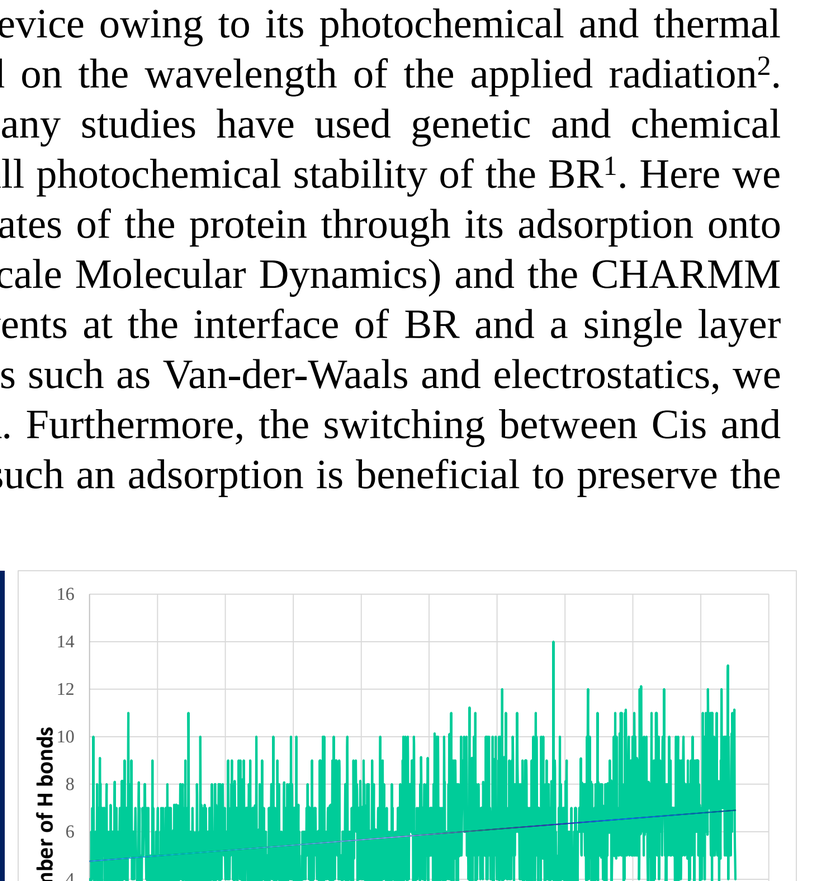

Figure 6: Secondary Structure of Protein for all frames.

CONCLUSION

- This study provides evidence that the BR protein can be immobilized onto graphene.
- Based on data from RMSD, salt bridges and interaction energy, it is found that BR after some molecular conformations have started to adsorb and stabilize.
- In future, this study aims to know about the cis and trans conformational stability of BR bound retinal on adsorption to graphene.

REFERENCES

1. Birge RR, Gillespie NB, Izaguirre EW, et al. *J Phys Chem B*. 1999;103(49):10746-10766. doi:10.1021/jp991883n.
2. Wagner NL, Greco J a, Ranaghan MJ, Birge RR. *J R Soc Interface*. 2013;10(84):20130197. doi:10.1098/rsif.2013.0197.
3. Humphrey W, Dalke A, Schulten K. *J Mol Graph*. 1996;14(1):33-38. doi:0263-7855(96)00018-5.
4. Jorgensen WL, Chandrasekhar J, Madura JD, Impey RW, Klein ML. *J Chem Phys*. 1983;79(2):926-935. doi:10.1063/1.445869.
5. Phillips JC, Braun R, Wang W, et al. *J Comput Chem*. 2005;26(16):1781-1802. doi:10.1002/jcc.20289.
6. MacKerell AD, Bashford D, Dunbrack RL, et al. *J Phys Chem B*. 1998;102(18):3586-3616. doi:10.1021/jp973084f.